

Title

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Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	C ₁₉ H ₁₂ FNO
M_r	289.30
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	6.3110 (1), 27.1770 (6), 8.6025 (2)
β (°)	107.089 (1)
V (Å ³)	1410.31 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.09
Crystal size (mm)	0.36 × 0.36 × 0.20
Data collection	
Diffractometer	Bruker APEX-II CCD
Absorption correction	Multi-scan Bruker-Nonius SADABS
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30761, 7836, 5645
R_{int}	0.023
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.874
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.051, 0.154, 1.04
No. of reflections	7836
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.43, -0.28

Computer programs: Bruker APEX2, Bruker SAINT, SHELXS2014 (Sheldrick, 2014), SHELXL2014 (Sheldrick, 2014), Bruker SHELXTL.

Acknowledgements

Funding information

References

Figure 1

supporting information

Title

Computing details

Data collection: Bruker *APEX2*; cell refinement: Bruker *SAINT*; data reduction: Bruker *SAINT*; program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2014); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2014); molecular graphics: Bruker *SHELXTL*; software used to prepare material for publication: Bruker *SHELXTL*.

1-(4-Fluorobenzoyl)-9H-carbazole

Crystal data

C₁₉H₁₂FNO
 $M_r = 289.30$
 Monoclinic, $P2_1/c$
 $a = 6.3110$ (1) Å
 $b = 27.1770$ (6) Å
 $c = 8.6025$ (2) Å
 $\beta = 107.089$ (1)°
 $V = 1410.31$ (5) Å³
 $Z = 4$
 $F(000) = 600$

$D_x = 1.363$ Mg m⁻³
 Melting point = 424–426 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 9948 reflections
 $\theta = 2.6$ – 36.3 °
 $\mu = 0.09$ mm⁻¹
 $T = 296$ K
 Irregular block, colourless
 $0.36 \times 0.36 \times 0.20$ mm

Data collection

Bruker APEX-II CCD
 diffractometer
 Radiation source: microfocus sealed tube
 φ and ω scans
 Absorption correction: multi-scan
 Bruker-Nonius *SADABS*

7836 independent reflections
 5645 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\text{max}} = 38.4$ °, $\theta_{\text{min}} = 2.9$ °
 $h = -11 \rightarrow 10$
 $k = -47 \rightarrow 42$
 $l = -15 \rightarrow 11$

30761 measured reflections

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.154$
 $S = 1.04$
 7836 reflections
 199 parameters
 0 restraints
 Primary atom site location: structure-invariant direct
 methods

Secondary atom site location: difference Fourier map
 Hydrogen site location: inferred from neighbouring
 sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0788P)^2 + 0.1787P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.43$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.28$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.8965 (1)	0.42021 (3)	0.08957 (9)	0.0245 (1)
H1A	0.9876	0.4407	0.0679	0.029*
C1	0.8810 (1)	0.37060 (3)	0.04960 (9)	0.0242 (1)
C2	1.0019 (2)	0.34351 (3)	−0.0326 (1)	0.0310 (2)
H2A	1.1134	0.3579	−0.0678	0.037*
C3	0.9488 (2)	0.29404 (4)	−0.0598 (1)	0.0376 (2)
H3A	1.0261	0.2750	−0.1147	0.045*
C4	0.7818 (2)	0.27225 (3)	−0.0066 (1)	0.0394 (2)
H4A	0.7497	0.2391	−0.0273	0.047*
C5	0.6632 (2)	0.29916 (3)	0.0764 (1)	0.0329 (2)
H5A	0.5529	0.2844	0.1121	0.039*
C6	0.7135 (1)	0.34912 (3)	0.10495 (9)	0.0242 (1)
C7	0.6251 (1)	0.38796 (3)	0.18232 (9)	0.0226 (1)
C8	0.4621 (1)	0.38949 (3)	0.2613 (1)	0.0274 (2)
H8A	0.3841	0.3612	0.2711	0.033*
C9	0.4171 (1)	0.43391 (3)	0.3255 (1)	0.0288 (2)
H9A	0.3078	0.4353	0.3780	0.035*
C10	0.5341 (1)	0.47636 (3)	0.3119 (1)	0.0255 (1)
H10A	0.5010	0.5055	0.3562	0.031*
C11	0.6999 (1)	0.47655 (3)	0.23356 (9)	0.0220 (1)
C12	0.7438 (1)	0.43130 (3)	0.16892 (9)	0.0211 (1)
C13	0.8358 (1)	0.52015 (3)	0.2273 (1)	0.0255 (1)
O1	0.9940 (1)	0.51718 (3)	0.1717 (1)	0.0401 (2)
C14	0.7901 (1)	0.56831 (3)	0.29520 (9)	0.0241 (1)
C15	0.5798 (2)	0.58970 (3)	0.2512 (1)	0.0286 (2)
H15A	0.4607	0.5731	0.1813	0.034*
C16	0.5472 (2)	0.63560 (3)	0.3110 (1)	0.0332 (2)
H16A	0.4083	0.6505	0.2799	0.040*
C17	0.7262 (2)	0.65857 (3)	0.4177 (1)	0.0327 (2)
F1	0.6923 (1)	0.70242 (2)	0.4815 (1)	0.0514 (2)
C18	0.9365 (2)	0.63876 (3)	0.4645 (1)	0.0322 (2)
H18A	1.0536	0.6553	0.5369	0.039*
C19	0.9688 (1)	0.59346 (3)	0.4004 (1)	0.0277 (2)
H19A	1.1100	0.5797	0.4276	0.033*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0247 (3)	0.0226 (3)	0.0285 (3)	−0.0022 (2)	0.0114 (2)	−0.0027 (2)
C1	0.0252 (3)	0.0221 (3)	0.0239 (3)	0.0020 (2)	0.0051 (2)	−0.0014 (2)
C2	0.0306 (4)	0.0299 (4)	0.0324 (4)	0.0066 (3)	0.0094 (3)	−0.0032 (3)
C3	0.0446 (5)	0.0281 (4)	0.0392 (5)	0.0118 (4)	0.0110 (4)	−0.0032 (3)
C4	0.0536 (6)	0.0204 (4)	0.0436 (5)	0.0050 (4)	0.0133 (4)	−0.0012 (3)
C5	0.0435 (5)	0.0212 (3)	0.0336 (4)	−0.0022 (3)	0.0107 (4)	0.0003 (3)
C6	0.0278 (3)	0.0208 (3)	0.0220 (3)	0.0003 (2)	0.0041 (2)	0.0003 (2)
C7	0.0233 (3)	0.0224 (3)	0.0211 (3)	−0.0023 (2)	0.0049 (2)	0.0000 (2)
C8	0.0269 (4)	0.0286 (4)	0.0276 (3)	−0.0074 (3)	0.0095 (3)	−0.0025 (3)
C9	0.0257 (3)	0.0336 (4)	0.0303 (4)	−0.0050 (3)	0.0133 (3)	−0.0044 (3)
C10	0.0255 (3)	0.0267 (3)	0.0252 (3)	−0.0005 (3)	0.0089 (3)	−0.0029 (3)

C11	0.0232 (3)	0.0216 (3)	0.0214 (3)	−0.0004 (2)	0.0070 (2)	−0.0010 (2)
C12	0.0215 (3)	0.0213 (3)	0.0202 (3)	−0.0007 (2)	0.0058 (2)	−0.0007 (2)
C13	0.0310 (4)	0.0216 (3)	0.0257 (3)	−0.0018 (3)	0.0113 (3)	−0.0009 (2)
O1	0.0481 (4)	0.0297 (3)	0.0546 (4)	−0.0098 (3)	0.0341 (4)	−0.0082 (3)
C14	0.0291 (3)	0.0203 (3)	0.0219 (3)	−0.0006 (2)	0.0058 (2)	0.0004 (2)
C15	0.0309 (4)	0.0244 (3)	0.0246 (3)	0.0019 (3)	−0.0010 (3)	−0.0006 (3)
C16	0.0354 (4)	0.0247 (4)	0.0336 (4)	0.0076 (3)	0.0009 (3)	0.0008 (3)
C17	0.0433 (5)	0.0179 (3)	0.0331 (4)	0.0021 (3)	0.0053 (3)	−0.0016 (3)
F1	0.0622 (5)	0.0229 (3)	0.0626 (5)	0.0053 (3)	0.0083 (4)	−0.0131 (3)
C18	0.0356 (4)	0.0228 (3)	0.0325 (4)	−0.0044 (3)	0.0011 (3)	−0.0016 (3)
C19	0.0276 (4)	0.0229 (3)	0.0303 (4)	−0.0018 (3)	0.0048 (3)	0.0014 (3)

Geometric parameters (Å, °)

N1—C12	1.368 (1)	C9—H9A	0.9300
N1—C1	1.388 (1)	C10—C11	1.401 (1)
N1—H1A	0.8600	C10—H10A	0.9300
C1—C2	1.394 (1)	C11—C12	1.410 (1)
C1—C6	1.407 (1)	C11—C13	1.473 (1)
C2—C3	1.389 (1)	C13—O1	1.231 (1)
C2—H2A	0.9300	C13—C14	1.495 (1)
C3—C4	1.398 (2)	C14—C15	1.396 (1)
C3—H3A	0.9300	C14—C19	1.399 (1)
C4—C5	1.385 (2)	C15—C16	1.388 (1)
C4—H4A	0.9300	C15—H15A	0.9300
C5—C6	1.400 (1)	C16—C17	1.378 (1)
C5—H5A	0.9300	C16—H16A	0.9300
C6—C7	1.444 (1)	C17—F1	1.355 (1)
C7—C8	1.390 (1)	C17—C18	1.378 (1)
C7—C12	1.419 (1)	C18—C19	1.388 (1)
C8—C9	1.391 (1)	C18—H18A	0.9300
C8—H8A	0.9300	C19—H19A	0.9300
C9—C10	1.393 (1)		
C12—N1—C1	109.22 (7)	C9—C10—C11	122.17 (8)
C12—N1—H1A	125.4	C9—C10—H10A	118.9
C1—N1—H1A	125.4	C11—C10—H10A	118.9
N1—C1—C2	129.03 (8)	C10—C11—C12	116.58 (7)
N1—C1—C6	108.91 (7)	C10—C11—C13	123.06 (7)
C2—C1—C6	122.05 (8)	C12—C11—C13	120.21 (7)
C3—C2—C1	117.12 (9)	N1—C12—C11	129.62 (7)
C3—C2—H2A	121.4	N1—C12—C7	108.89 (7)
C1—C2—H2A	121.4	C11—C12—C7	121.48 (7)
C2—C3—C4	121.51 (9)	O1—C13—C11	120.61 (7)
C2—C3—H3A	119.2	O1—C13—C14	118.75 (7)
C4—C3—H3A	119.2	C11—C13—C14	120.59 (7)
C5—C4—C3	121.24 (9)	C15—C14—C19	119.56 (7)
C5—C4—H4A	119.4	C15—C14—C13	122.40 (7)
C3—C4—H4A	119.4	C19—C14—C13	117.97 (8)
C4—C5—C6	118.27 (9)	C16—C15—C14	120.45 (8)
C4—C5—H5A	120.9	C16—C15—H15A	119.8
C6—C5—H5A	120.9	C14—C15—H15A	119.8

C5—C6—C1	119.81 (8)	C17—C16—C15	118.18 (8)
C5—C6—C7	133.72 (8)	C17—C16—H16A	120.9
C1—C6—C7	106.45 (7)	C15—C16—H16A	120.9
C8—C7—C12	119.94 (7)	F1—C17—C16	118.17 (9)
C8—C7—C6	133.53 (7)	F1—C17—C18	118.58 (8)
C12—C7—C6	106.53 (7)	C16—C17—C18	123.25 (8)
C7—C8—C9	119.10 (7)	C17—C18—C19	118.14 (8)
C7—C8—H8A	120.4	C17—C18—H18A	120.9
C9—C8—H8A	120.4	C19—C18—H18A	120.9
C8—C9—C10	120.72 (8)	C18—C19—C14	120.38 (8)
C8—C9—H9A	119.6	C18—C19—H19A	119.8
C10—C9—H9A	119.6	C14—C19—H19A	119.8
